What is claimed is:

1. A computer-based method of generating a quantitative structure activity relationship comprising:

a) calculating a numerical representation of molecules consisting of *n* numbers per molecule; and,

b) estimating a probability distribution that *a* said molecules is active.

2. A method as recited in claim 1, wherein:

a) said estimating step is calculated with Bayes Theorem.

3. A method as recited in claim 1, wherein:

a) said probability distribution of said estimating step comprises *n* one-dimensional distributions.

4. A method as recited in claim 1, wherein:

a) said estimating step is performed by using a means to remove linear correlations between said *n* numbers per molecule.

5. A method as recited in claim 4, wherein:

a) said means to remove linear correlations between said *n* numbers per molecule is a principal components analysis.

6. A method as recited in claim 4, wherein:

a) said means to remove linear correlations between said *n* numbers per molecule is a matrix diagonalization.

7. A method as recited in claim 1, wherein:

a) said estimating step is performed by using a means to remove dependencies between said *n* numbers per molecule.

8. A method as recited in claim 7, wherein:

a) said means to remove dependencies between said *n* numbers per molecule is a principal components analysis.

9. A method as recited in claim 7, wherein:

a) said means to remove dependencies between said *n* numbers per molecule is a matrix diagonalization.

10. A method as recited in claim 1, wherein:

a) said estimating step is performed by estimating a distribution over a single number.

11. A method as recited in claim 1, wherein:

a) said estimating step is performed by replacing a single observation with a Gaussian distribution.